Mobile Bipolarons in the Adiabatic Holstein-Hubbard Model in 1 and 2 dimensions.

L. Proville and S. Aubry [1,2]

Laboratoire Léon Brillouin (CEA-CNRS), CE Saclay
91191-Gif-sur-Yvette Cedex, France

Abstract

The bound states of two electrons in the adiabatic Holstein-Hubbard model are studied numerically in one and two dimensions from the anticontinuous limit. This model involves a competition between a local electron-phonon coupling (with a classical lattice) which tends to form pairs of electrons and the repulsive Hubbard interaction $U \geq 0$ which tends to break them.

In 1D, the ground-state always consists in a pair of localized polarons in a singlet state. They are located at the same site for $U = 0$. Increasing U, there is a first order transition at which the bipolaron becomes a spin singlet pair of two polarons bounded by a magnetic interaction. The pinning mode of the bipolaron soften in the vicinity of this transition leading to a higher mobility of the bipolaron which is tested numerically.

In 2D, and for any U, the electron-phonon coupling needs to be large enough in order to form small polarons or bipolarons instead of extended electrons. We calculate the phase diagram of the bipolaron involving first order transitions lines with a triple point. A pair of polarons can form three types of bipolarons: a) on a single site at small U, b) a spin singlet state on two nearest neighbor sites for larger U as in 1D and c) a new intermediate state obtained as the resonant combination of four 2-sites singlet states sharing a central site, called quadrisinglet.

The breathing and pinning internal modes of bipolarons in 2D generally only weakly soften and thus, they are practically not mobile. On the opposite, in the vicinity of the triple point involving the quadrisinglet, both modes exhibit a significant softening. However, it was not sufficient for allowing the existence of a classical mobile bipolaron (at least in that model).

[1] email: proville@bali.saclay.cea.fr
[2] email: aubry@bali.saclay.cea.fr

1 Introduction

It is well-known for many decades since [1] that a single electron submitted to an electron phonon coupling may generate a polaron that is a quasi-particle consisting into an electron localized in a self consistent lattice potential. For a local electron phonon interaction, the formation of a polaron always occurs in 1D. At small coupling, this polaron becomes large and highly mobile. On the opposite, in 2D (and more dimensions), the formation of a polaron requires a large enough coupling [2]. Then, the polarons are always small that is mostly localized on a single site and not mobile.

If there is no electron repulsion, two polarons form a bipolaron with two electrons in a spin singlet state localized in the same potential well. When there is a strong enough electronic repulsion, the bipolaron may be broken into two unbound polarons. However, in the intermediate regime, we are going to show that there are new bounded bipolaronic states with interesting properties.

There have been many tentative theories about bipolaronic superconductivity for many years (see [4] for a review). In the well-known BCS theory valid at weak electron phonon coupling, the electron pairs (Cooper pairs) form self consistently in the superconducting phase only and are spatially very extended. For the bipolaronic superconductivity, it is speculated that when there are pre-existent bounded pairs of electrons (small bipolaron), that they may behave as a quantum boson liquid and condense into a superfluid state. However, the most serious critiscismes to these theories is that when the bipolarons exist in 2 and 3 D models (with realistic physical parameters), their effective mass is so huge that their quantum character completely disappear. They should condense into spatially ordered or disordered structures which could be just considered as a chemical bond ordering.

Expansions at large electron phonon coupling [3], modelize the bipolaronic system as an array of coupled quantum spins 1/2 with two types of coupling. The spin is $+1/2$ at a site occupied by a bipolaron and $-1/2$ in the opposite case. There is an $x-y$ coupling between neighboring spins describing the bipolaron tunnelling and which yields the bipolaron band width and a $z-z$ coupling representing the potential interaction between the bipolarons. If the $x-y$ term dominates, the spin ordering occurs in the plane $x-y$ and the structure is superconducting. If the z term dominates, one get a spatial ordering of the pseudospin in the z direction that is a spatial ordering of the bipolarons (or chemical bonds) in the real space. The real systems where the effective mass of the electrons are usually much smaller than the atomic masses are generally close to the adiabatic limit. In that case the $x-y$ couplings turns out to be negligible compared to the z interaction which eliminates any possibility of superconductivity but instead of, a spatial bipolaron ordering.

It is clear that this regime is quite well-described within a purely adiabatic approximation (the *chemist* approximation).

However, it might exist special situations where this $x-y$ coupling could be enhanced to relative large values and dominates the z coupling thus favoring a bipolaronic superconductivity at unusually high temperatures. The purpose of this paper is to show that in a restricted region of the parameter space only, the competition between the electron phonon coupling and the electron-electron repulsion could produce a sharp increase in the mobility of bipolarons while simultaneously the binding energy of the bipolaron remains significantly large thus favoring superconductivity as conjectured in [7,10].

We test these ideas on the simplest model which is the Holstein Hubbard model, where both electron-phonon interactions and electron-electron interaction are involved. In a first step, we consider the adiabatic model where the quantum fluctuations of the lattice are neglected and shall look at the bipolaron classical mobility only. The next step will be done in a forthcoming work, where it will be shown that when the bipolarons are very mobile, the adiabatic approximation is not valid because they are very sensitive to the quantum lattice fluctuation by producing a sharp increase of the bipolaron bandwidth.

2 The Model: definitions

In order to make the physical parameters explicit, we write the Holstein-Hubbard Hamiltonian with its full set of parameters:

$$\mathcal{H} = -T \sum_{<i,j>,\sigma} C^{+}_{i,\sigma} C_{j,\sigma} + \sum_{i} \hbar\omega_0 (a^{+}_{i} a_i) + g n_i (a^{+}_{i} + a_i) + \upsilon n_{i,\uparrow} n_{i,\downarrow} \quad (1)$$

where T is the transfer integral between nearest neighbor sites $< i,j >$ of the lattice, of the electrons represented by the standard fermion operators $C^{+}_{i,\sigma}$ and $C_{j,\sigma}$ at site i with spin $\sigma =\uparrow$ or $\downarrow$. a^{+}_{i} and a_i are standard creation and annihilation boson operators of phonons. $\hbar\omega_0$ is the phonon energy of a dispersionless optical phonon branch. g is the constant of the onsite electron phonon coupling. The onsite electron-electron interaction is represented by a Hubbard term with positive coupling υ.

Choosing the energy $E_0 = 8g^2/\hbar\omega_0$ as energy unit and introducing the position and momentum operators:

$$u_i = \frac{\hbar\omega_0}{4g}(a^{+}_{i} + a_i) \quad (2)$$

$$p_i = i\frac{2g}{\hbar\omega_0}(a_i^+ - a_i) \tag{3}$$

we obtain the dimensionless hamiltonian:

$$H = \sum_i \left(\frac{1}{2}u_i^2 + \frac{1}{2}u_i n_i + U n_{i\uparrow} n_{i\downarrow}\right) - \frac{t}{2}\sum_{<i,j>,\sigma} C_{i,\sigma}^+ C_{j,\sigma} + \frac{\gamma}{2}\sum_i p_i^2 \tag{4}$$

The parameters of the system are now:

$$E_0 = 8g^2/\hbar\omega_0 \qquad U = \frac{\upsilon}{E_0} \qquad t = \frac{T}{E_0} \qquad \gamma = \frac{1}{4}(\frac{\hbar\omega_0}{2g})^4 \tag{5}$$

As soon as the electron phonon coupling g becomes reasonably large that is larger than the phonon energy $\hbar\omega_0$, γ becomes very small. The adiabatic approximation is obtained by taking $\gamma = 0$. We shall assume this condition from nowon.

Then $\{u_i\}$ commutes with the Hamiltonian and can be taken as a scalar variable. For a given set of $\{u_i\}$, the 2-electron ground-state of the Hamiltonian

$$H_{ad} = \sum_i \left(\frac{1}{2}u_i^2 + \frac{1}{2}u_i n_i + U n_{i\uparrow} n_{i\downarrow}\right) - \frac{t}{2}\sum_{<i,j>,\sigma} C_{i,\sigma}^+ C_{j,\sigma} \tag{6}$$

has to be searched among singlet states with the form

$$|\Psi> = \sum_{i,j} \psi_{i,j} C_{i,\uparrow}^+ C_{j,\downarrow}^+ |\emptyset> \tag{7}$$

where $\psi_{i,j} = \psi_{j,i}$ is normalized $\sum_{i,j} |\psi_{i,j}|^2 = 1$. Then the energy of the system depends on $|\psi> = \{\psi_{i,j}\}$ and $\{u_i\}$ as

$$F(\{\psi_{i,j}\}, \{u_i\}) = \sum_i \left(\frac{1}{2}u_i^2 + u_i\rho_i + U|\psi_{i,i}|^2\right) - \frac{t}{2} < \psi|\Delta|\psi > \tag{8}$$

where

$$\rho_i = \frac{1}{2}\sum_j (|\psi_{i,j}|^2 + |\psi_{j,i}|^2) \tag{9}$$

is the half electronic density at site i and Δ is a discrete Laplacian operator in $2d$ dimensions (d being the initial lattice dimension).

3 The anticontinuous limit

The minimization of $F(\{\psi_{i,j}\},\{u_i\})$ with respect to the normalized electronic state $\{\psi_i^*\}$ yields the electronic eigenequation

$$-\frac{t}{2}\Delta\psi_{i,j}+\left(\frac{1}{2}(u_i+u_j)+U\delta_{i,j}\right)\psi_{i,j}=F_{el}(\{u_i\})\psi_{i,j} \tag{10}$$

where F_{el} is the electronic ground-state energy in the potential generated by $\{u_i\}$. Then for $t>0$, the wave function $\psi_{i,j}$ has to be real, positive and symmetric. The adiabatic potential for the atoms is then

$$F_{ad}(\{u_i\})=\sum_i\frac{1}{2}u_i^2+F_{el}(\{u_i\}) \tag{11}$$

It has infinitely many minima [6,8,11] close to the anticontinuous limit $t=0$. An adiabatic configuration $\{u_i\}$ is metastable when it is a local minima of 11 [6].

The minimization of $F(\{\psi_{i,j}\},\{u_i\})$ can also be done first with respect to $\{u_i\}$ which yields $u_i+\rho_i=0$. Substitution in 8, yields a different variational form on $\{\psi_{i,j}\}$ non equivalent to 11

$$F_\psi(\{\psi_{i,j}\},\{u_i\})=\sum_i\left(-\frac{1}{2}\rho_i^2+U\sum_i|\psi_{i,i}|^2\right)-\frac{t}{2}<\psi|\Delta|\psi> \tag{12}$$

The extremalization of 12 with respect to $\psi_{i,j}$ with the condition of normalization, yields a generalized discrete nonlinear Schroedinger equation on a $2d$-dimensional lattice

$$-\frac{t}{2}\Delta\psi_{i,j}+\left(-\frac{1}{2}(\rho_i+\rho_j)+U\delta_{i,j}\right)\psi_{i,j}=F_{el}\psi_{i,j} \tag{13}$$

corresponding to 10.

This equation 13 has also an anticontinuous limit at $t=0$ which is different of those of model 11. It yields more states at this limit because it is not required that the electronic eigen states be in its ground-state with respect to the lattice potential. This allows one to involve electronic excitations but it has of course the same ground-states. The classification of these states will not be discussed here.

However for eq.13 at $t=0$, the phases of each complex number $\psi_{i,j}$ is arbitrary. This situation is analogous to the anticontinuous limit of the breather problem

where the phase of the uncoupled oscillators is degenerate (see ref.[12,13] for details). The consequence is that the implicit function theorem cannot be applied directly for proving the possible continuation of the solutions at $t = 0$. For the breather problem, a trick has been to consider first only time reversible solutions thus removing this phase degeneracy but this was not absolutely necessary [13,14]). In our model, it is also convenient to consider in a first step only real electronic wave functions. Then, these real normalized solutions at $t = 0$ can be continued for $t \neq 0$ not too large. This is not a restriction for finding the electronic ground-states because we know that the corresponding electronic state is real, positive and symmetric.

This continuation can be done by numerical methods. Most of the real solutions of 13 are unstable for t small but some of them can recover stability at larger t and even become the ground-state. We calculated numerically with a high accuracy a few number of these solutions rather well localized on a small number of sites (also taking advantage of its spatial symmetries if any) which we believed to be possible candidate for being a ground-state. By comparing their energies one with each others, the bipolarons state are found which are presumably the exact ground-state. In the domain of parameter we explored, we found mostly three kinds of bipolaronic states with a significantly large binding energy (see fig.1) as ground-states in some domain of U and t. [3] They are obtained by continuation from the following solutions of eq. 13 at $t = 0$:

1-the standard onsite bipolaron denoted (S0) at given site i where

$$\psi_{i,i} = 1 \quad \text{and} \quad \psi_{m,n} = 0 \quad \text{else for} \quad (m,n) \neq (i,i) \tag{14}$$

2- the two-site singlet bipolaron , localized on two nearest neighbor sites i and j denoted (S1) which was named "Spin Resonant" bipolaron in ref.[7,10]. We also observed ground-states which are singlet states where the polarons are at distance 2 (denoted (S2) but with a weaker binding energy.

$$\begin{aligned} &\psi_{i,j} = \psi_{j,i} = \frac{1}{\sqrt{2}} \quad \text{and} \\ &\psi_{m,n} = 0 \quad \text{else for} \quad (m,n) \neq (i,j) \quad \text{and} \quad (m,n) \neq (j,i) \end{aligned} \tag{15}$$

3-and in two dimensions, a new unexpected solution which is the quadrisinglet localized bipolaron denoted (QS) which is localized at the given site i and its

[3] However, there are unexplored domains for large U where the ground-states will be different but their very weak binding energy makes that they are less interesting at the present stage of our approach.

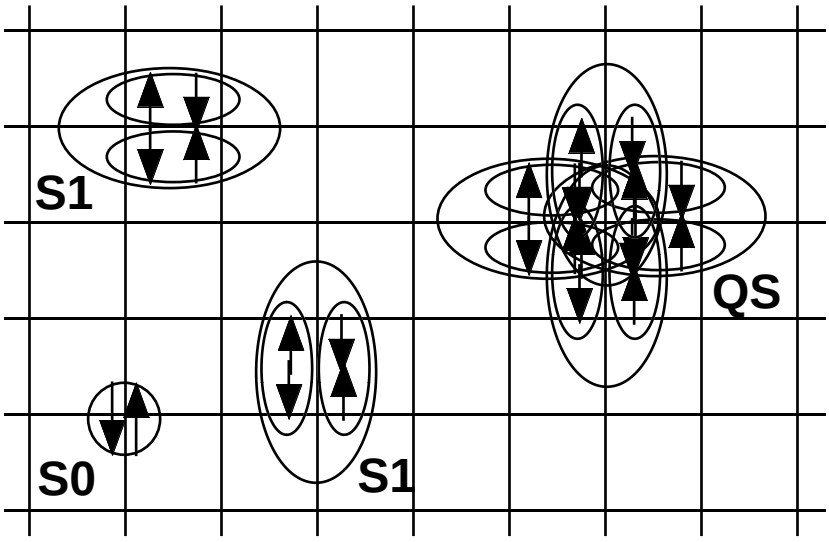


Fig. 1. Schemes representing on a 2d lattice a) a standard onsite bipolaron (S0) b) two-site singlet bipolarons ("Spin Resonant Bipolaron") (S1) in x and y directions c) a quadrisinglet bipolaron localized on four bonds (QS).

four nearest neighbors j_ν ($\nu = 1, .., 4$). It is the linear combination of four singlets located on the four nearest neighbor bonds $< i, j_\nu >$

$$\begin{aligned} &\psi_{i,j_\nu} = \psi_{j_\nu,i} = \frac{1}{\sqrt{8}} \quad \text{and} \\ &\psi_{m,n} = 0 \quad \text{else for} \quad (m,n) \neq (i,j_\nu) \quad \text{and} \quad (m,n) \neq (j_\nu,i) \end{aligned} \tag{16}$$

This solution can be viewed as a localized RVB state similar to those proposed by Anderson some years ago [5] in the pure Hubbard model in 2D as a theory for superconductivity in cuprates. The physical origin of the binding of the bipolaron in states (S1), (S2).. and (QS) can be interpreted of magnetic origin. When the Hubbard term increases too much, bipolaron (S0) could break into two polarons far apart but then both of them are magnetic with a spin 1/2. They should interact by an antiferromagnetic exchange coupling, as predicted by standard perturbation theories. Then, for moderately large Hubbard terms, it remains more favorable to reduce the distance between the two polarons for gaining a magnetic energy by forming a singlet state (S1), (S2).... We have no simple interpretation to explain why bipolaron (QS) which has a more complex structure and could become the most stable in 2D models but is not in 1D (as far in our domains of investigation).

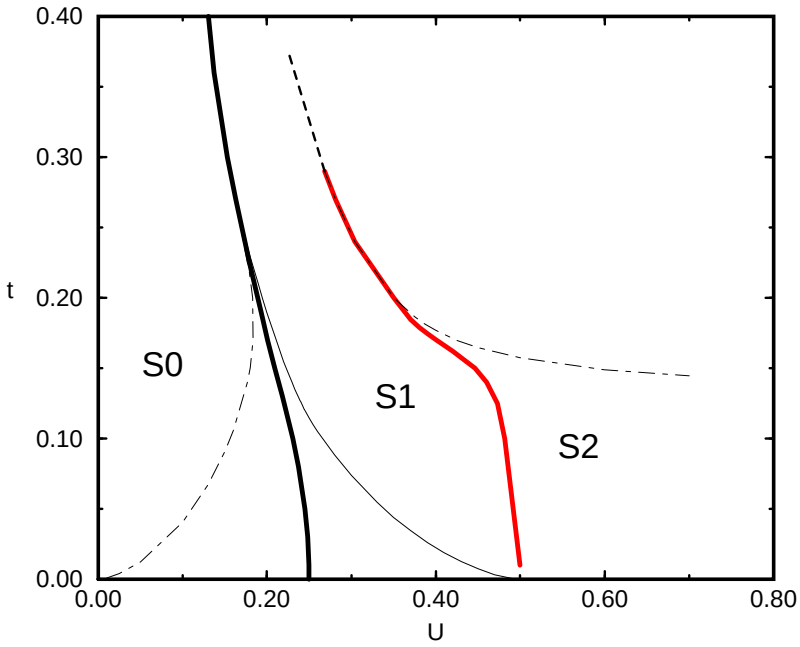


Fig. 2. Phase diagram versus U and t of the bipolaronic ground-state. showing first order transition lines (solid lines) between bipolarons (S0) and (S1) and between bipolarons (S1) and (S2). The thin line is the limit of metastability of bipolaron (S0) and the two dot-dashed lines are those of (S1).

4 Bipolaronic Ground-states in One dimension

The size of the system was chosen large enough compared to the bipolaron size (in our calculations up to the size 41 for spatially symmetric states). As expected, we found that for any value of t (tested up to $t = 0.6$), there is always a biplaronic state which is lower in energy than a pair of extended electrons. The phase diagram is shown fig.2.

The first order transition lines are sharp and well defined for t small when the bipolarons have a small spatial extension. When t increases, the size of the bipolarons also increases and it becomes practically impossible to distinguish numerically the energy differences between bipolaronic states obtained by continuation from different states at the anticontinuous limit. This can be interpreted by the fact that when t is large, such a model is well described with a continuous space variable x instead of the discrete lattice site i. This continuous model exhibit only one bipolaronic solution which "erases" all the transitions due to discreteness.

We now look at the possible mobility of the obtained bipolarons. The precise

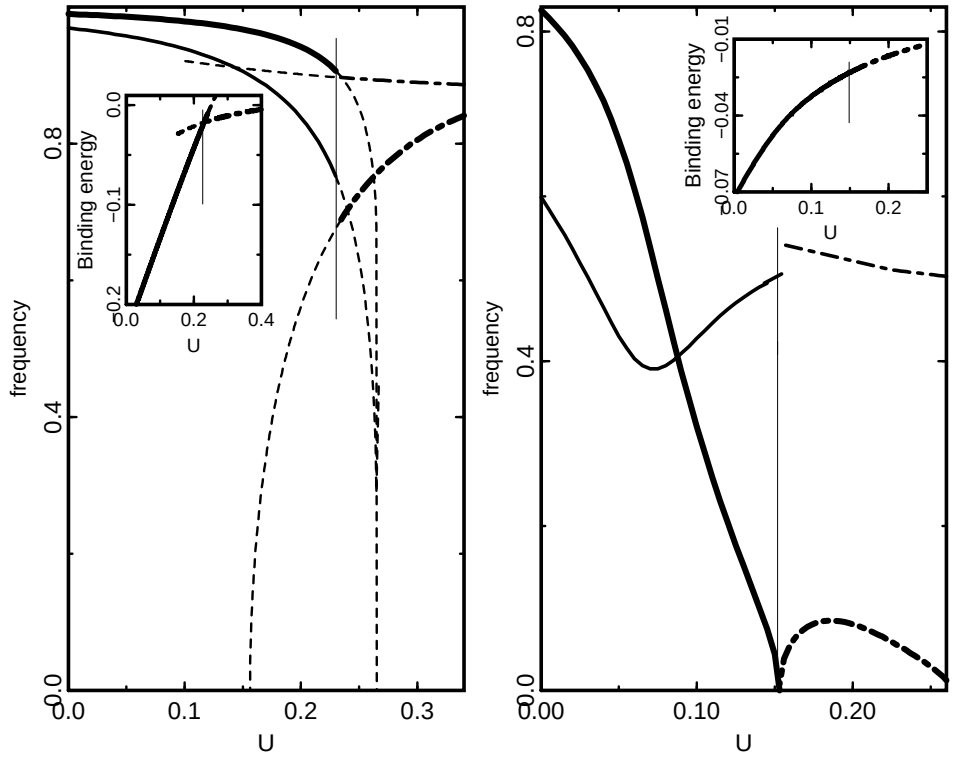


Fig. 3. Frequencies versus U of the pinning modes (thick lines) and the breathing modes (thin lines) for bipolarons (S0) (full lines) and (S1) (dot-dashed lines) at $t = 0.1$ (left) and $t = 0.3$ (right). The inserts show the corresponding binding energies for breaking the bipolarons into two polarons far apart.

calculation of the Peierls-Nabarow(PN) energy barrier requires too much numerical work while the calculation of the pinning modes of the bipolarons is much easier and brings nevertheless a similar information. The eigenvalues of the matrix of the second variation of the lattice potential energy $F_{ad}(\{u_i\})$ 11 are the squares of the phonon frequencies of the bipolaron calculated within the standard Born-Oppenheimer approximation (in unit $\sqrt{\gamma}$). Beside the initial flat optical branch of phonon at frequency 1, there are two localized mode. One is spatially antisymmetric and correspond to the pinning mode of the bipolaron. The second one is spatially symmetric and is a breathing mode. There is a phonon softening at the first order transition between bipolaron (S0) and (S1) which becomes almost complete for t large enough. Fig.3 shows for $t = 0.3$, that the frequency of the bipolaron (S0) practically vanishes at the transition with (S1) which becomes almost second order.

A strong softening of the pinning mode of the bipolaron is usually associated with a high mobility. This can be tested by integrating the classical dynamical equations of the lattice with the effective potential $F_{ad}(\{u_i\})$ taking as initial condition the bipolaron configuration with a small perturbation in the direction of the pinning mode (see a similar calculation for a moving breather in ref.[15]). The moving bipolaron shown fig.4 corresponds to the dip of the

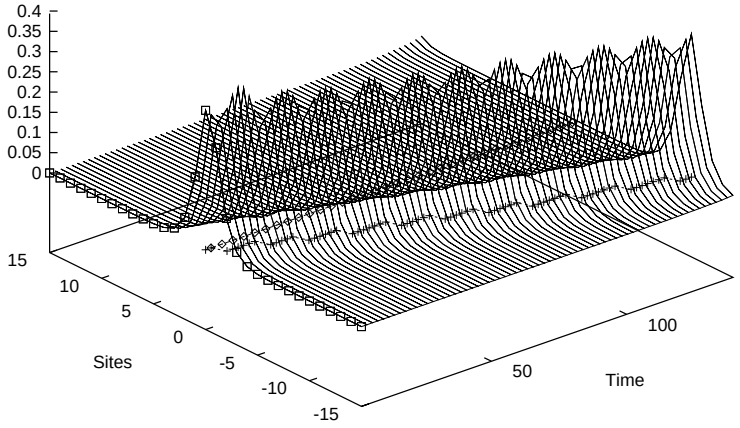


Fig. 4. 3D Plot of the electronic density $\{\rho_i\}$ versus time for a moving bipolaron (S0) at $t = 0.3$ and $U = 0.14$ ($\omega_p = 0.1$ and $\omega_b = 0.48$). See the projection of the density maximum showing the bipolaron motion.

pinning mode of fig.3. Although it is often believed that a high mobility for a localized object in discrete lattice can be achieved only when the size of this object is large compared to the lattice spacing, this moving bipolaron shown is localized on few sites only and also still strongly bounded (see inserts of fig.3). It is nevertheless highly mobile. During the motion, it can be viewed as exchanging from state (S0) to (S1) and vice-versa.

Relatively small perturbation of the model parameters suffices to raise the frequency of the pinning mode and then, it can be checked that the quality of the bipolaron mobility diminishes and progresively disappears.

5 Bipolaronic Ground-states in Two dimensions

In the 2D model, a smaller size (up to 14×14) for the lattice turns out to be sufficient for accurate calculations because the polaronic states remains quite localized while they exist.

The obtained phase diagram is shown fig.5. For t large enough, the ground-state corresponds to extended electrons. For t small, there is a first order transition as in the 1D model, between bipolarons (S0) and (S1) but also in addition, there is a small domain where the bipolaron (QS) which was initially unstable for t small, recover its stability and even becomes the ground-state.

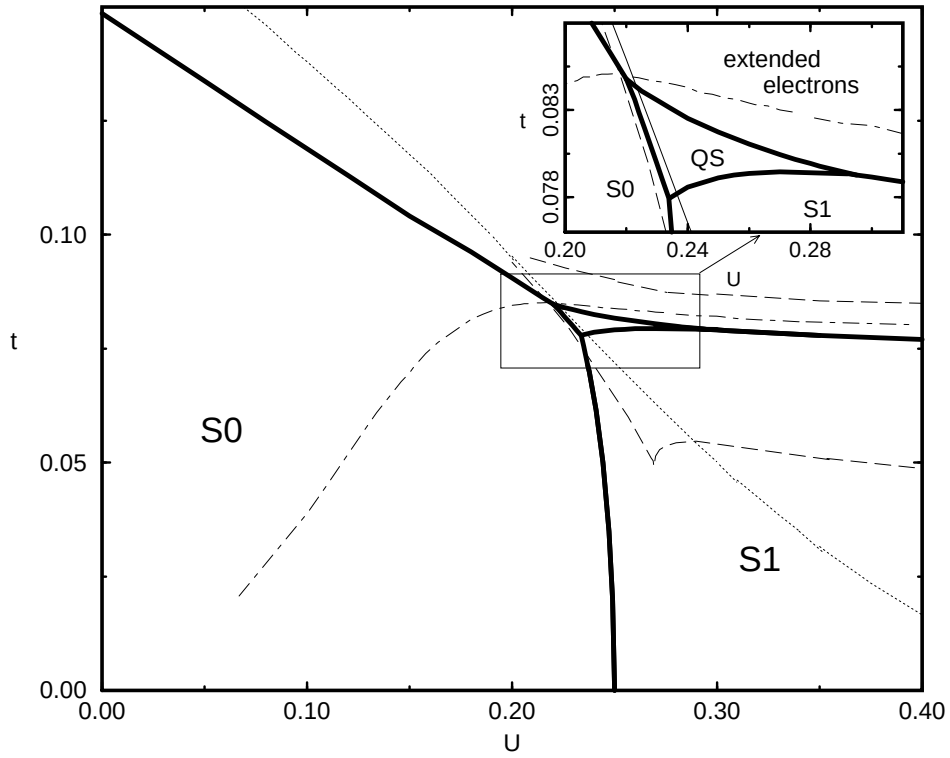


Fig. 5. Phase diagram versus U and t of the bipolaron in the 2D Holstein-Hubbard model with four phases separated by first order transition lines corresponding to bipolarons (S0), (S1), (QS) and extended electrons. The thin dotted line is the limit of metastability of bipolaron(S0), the dot-dashed line is the one of (S1) and the dashed lines are those of (QS). Insert: Magnification of the region of fig.5 around the triple point between phases (S0), (S1) and (QS).

The profiles of the three types of coexisting bipolarons (S0), (S1) and (QS) with a rather small spatial extension, are shown fig.6.

Insert fig. 7 shows the energies of the bipolarons on several lines at constant t. Although, it becomes relatively small, the bipolaron binding energies remains non negligible in the vicinity of the triple point.

As in 1D, the PN energy barrier is likely depressed in the vicinity of the first order transition line between (S0) and (S1) or (QS) and (S1) but difficult to calculate accurately. By contrast, the pinning and breathing frequencies of the bipolarons are much easier to calculate and shown fig.7 as a function of U for several values of t. For (S0) and (QS) there are two degenerate pinning modes, one corresponding to the x direction and the other one to the y direction. Fig.7 shows that there is significant softening of both the pinning modes and the breathing mode essentially in the vicinity of the triple point. However, this softening is not sufficient for allowing the bipolaron mobility in that region (as confirmed by our tests). One may consider that a model involving onsites couplings does not favor the bipolaron mobility. Further studies on

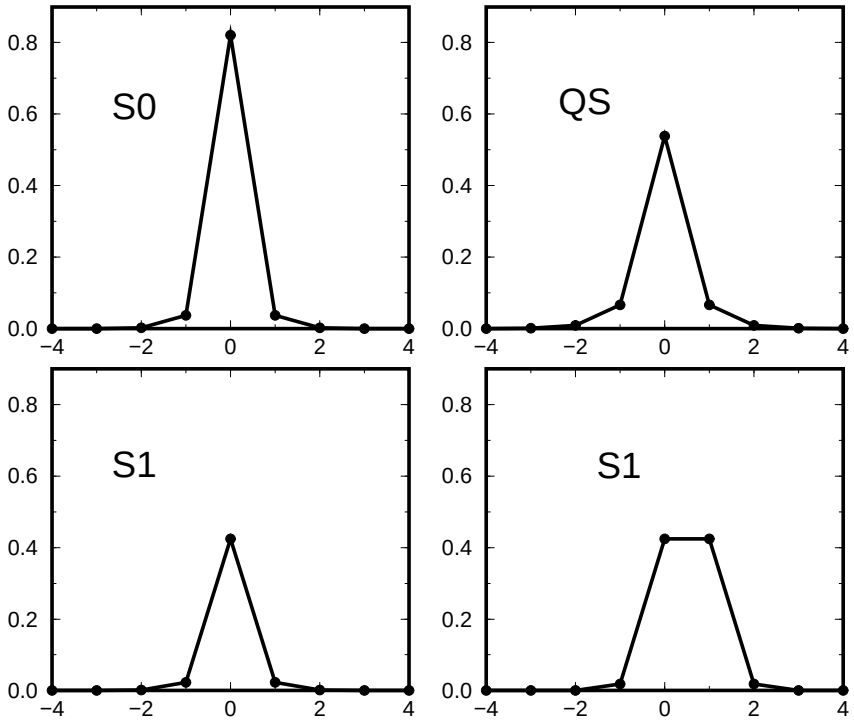


Fig. 6. Electronic density profiles versus site i at the triple point $t = 0.0779$, $U = 0.234$ for the bipolarons (S0), (QS) along the symmetry x axis and the profiles of (S1) along the symmetry x-axis and the transverse y-axis. These three bipolarons have the same energy.

modified Holstein-Hubbard models and particularly models chosen in order to approach a better description of the cuprates layers $Cu0_2$, could perhaps produce classically mobile bipolarons in $2D$.

6 Discussion and Concluding Remarks

Our results are not restricted to the original Holstein-Hubbard model. We already found that the three types of bipolarons (S0), (S1) and (QS) persist in appropriate domain of parameters for modified Holstein-Hubbard models for example when introducing nearest neighbour Hubbard interaction. We believe that few changes in the model which could be physically realistic, could favor the classical mobility. For example, a phonon dispersion chosen with an appropriate sign, should increases moderately the spatial extension of the bipolarons and thus favor its classical mobility.

In any case, although the classical mobility of a bipolaron should favor its quantum mobility, this condition is not necessary. When the quantum lattice fluctuation are taken into account ($\gamma \neq 0$ in eq.4, the quantum correction

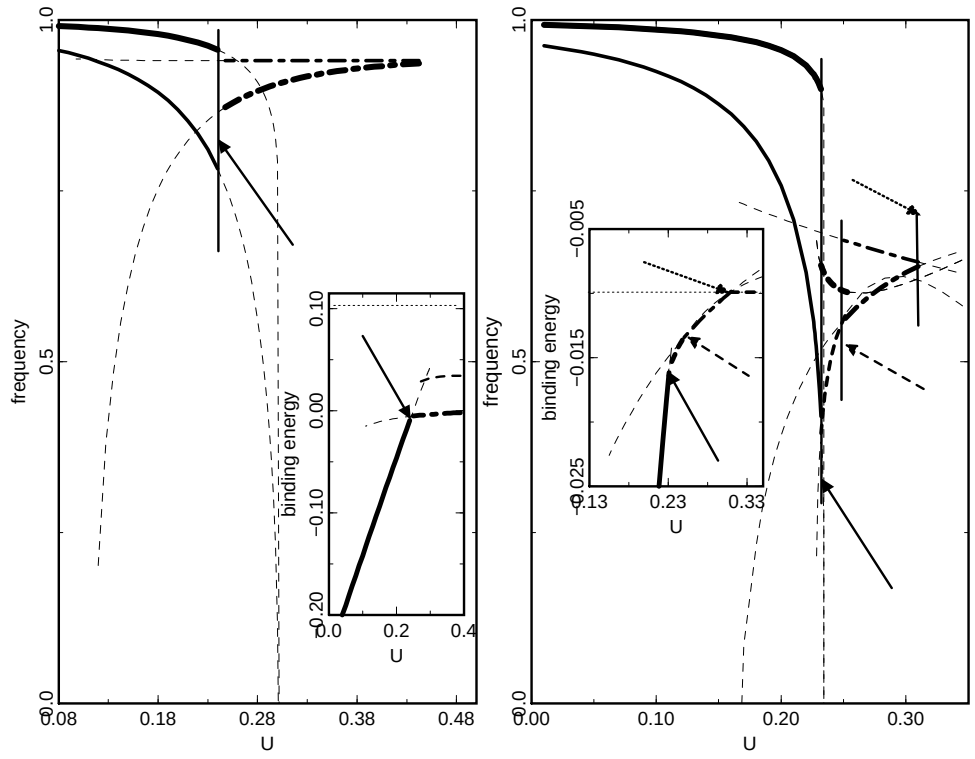


Fig. 7. Frequencies versus U of the pinning modes (thick lines) and the breathing modes (thin lines) for bipolarons (S0) (full lines), (S1) (dot-dashed lines)and (QS) (dashed lines) at $t = 0.05$ (left) and $t = 0.0791$ (right). The inserts show the corresponding binding energies for breaking the bipolarons into two polarons far apart. Arrows show the first order transitions and horizontal line is energy of extended electrons.

to the bipolaronic solutions should involve at the lowest order a RPA term (corresponding to small local quantum fluctuations) and the most important term concerning its physical consequences, a tunnelling term raising the spatial degeneracy of the bipolarons. The bipolarons should thus form bands.

Approximate methods for calculating these bands width analogous to those developped in ref.[16,17] can be used. In the vicinity of the triple point of the phase diagram 6, the three types of bipolarons (S0), (S1), (QS) have the same energies and are resonant. There are four hybridized bands associated with a sharp increase of each bandwidth with relatively small gaps for moderately small γ which makes globally a broad band while elsewhere the quantum mobility of the bipolarons sharply diminish. This current work shall be described in a forthcoming publication [18].

Although we only considered two electrons in the lattice, we could expect reasonably that a high bipolaron mobility could persist at finite density provided it remains sufficiently far from the half filled band. Approaching this limit, the hard core interaction should prevent this mobility and produce a frozen structure of polaron (likely a SDW or an antiferromagnet).

Before ending this paper, let us briefly check the physical relevance of our results. These preliminary studies indicates that although relatively weak, the binding energies of the bipolarons (for producing two extended polarons) in the vicinity of the triple point are about 0.005 with our energy unit E_0. This chemical energy has to be measured in eV as well as the Hubbard term (which is about 8eV for the ion Cu^{++}). Thus it is not unreasonable that this binding energy range within several 10^{-1} eV which is comparable to the critical temperature energies of the cuprates.

In summary, we found that in the 1D model when U increases from zero, the bipolarons are pairs of polarons at distance 0 (onsite bipolaron (S0), at distance 1 (two-sites bipolaron or Spin Resonant Bipolaron) (and further but with a binding energy going to zero very fast) and that there is first order transitions between these different configurations. In the 2D model, we find again the onsite bipolarons (S0) and the 2-site bipolaron (S1) but a new kind of bipolaron called quadrisinglet. There is a triple point in the phase diagram where the three kinds of bipolarons have the same energy. There is a significant phonon softening at the first order transition. In 1D, this softening can become almost complete at moderately large values of the transfer integral. Then, the classical bipolaron mobility has been effectively observed by direct simulation. By contrast, in 2D, the phonon softening has not been found sufficient to produce the classical mobility, but nevertheless one can expect a sharp effect of the bipolaron resonance at the triple point, when the quantum lattice fluctuations are taken into account.

We also bring more arguments which maintain our early conjectures [7,10]that the possible origin of high T_c superconductors originate from an exceptional combination of circonstances consisting in a well-balanced competition between strong repulsive electron-electron interactions and a strong electron-phonon interactions.

References

[1] L. Landau, 1933, Phys. Z. Sowjet, **3** 664

[2] D. Emin and T. Holstein, 1976, Phys.Rev.Letts **36** 323 and
D. Emin, 1982, Physics Today, June 1982 p.34

[3] A.S. Alexandrov, J. Ranninger and S. Robaszkiewicz,1986, Phys.Rev. **B33** 4526

[4] *Polarons and Bipolarons in High Tc Superconductors and related materials*, Ed. E.K.H. Salje, A.S. Alexandrov and W.Y.Liang, ,1995, Cambridge University Press

[5] P.Anderson, Science **235** (1987)1196
P.Anderson, G.Baskaran, Z.Zou and T.Hsu, Phys.Rev.Letts. **58**(1987) 2790-93

[6] S.Aubry, G.Abramovici and J.L. Raimbault, J. Stat. Phys. **67** 675-780 (1992)

[7] S. Aubry, in *Phase separation in Cuprate Superconductors* Ed. K.A.Müller and G.Benedek, World Scientific Pub. (the Science and Culture Series-Physics) (1993) p. 304-334

[8] S.Aubry, J.Physique IV colloque (Paris) **C2 3** (1993) 349-355

[9] S. Aubry, Physica **71D**(1994) 196-221

[10] S.Aubry, in *Polarons and Bipolarons in High Tc Superconductors and related materials* Ed. E.K.H. Salje, A.S. Alexandrov and W.Y.Liang, Cambridge University Press (1995) p. 271-308

[11] C. Baesens, R.S. MacKay, Nonlinearity **7** (1994) 59-84

[12] R.S. MacKay and S. Aubry, Nonlinearity**7** (1994) 1623-43

[13] S. Aubry, 1997, in *Lattice Dynamics* Eds. M. Courbage and H. Chaté, Physica **103D** in print

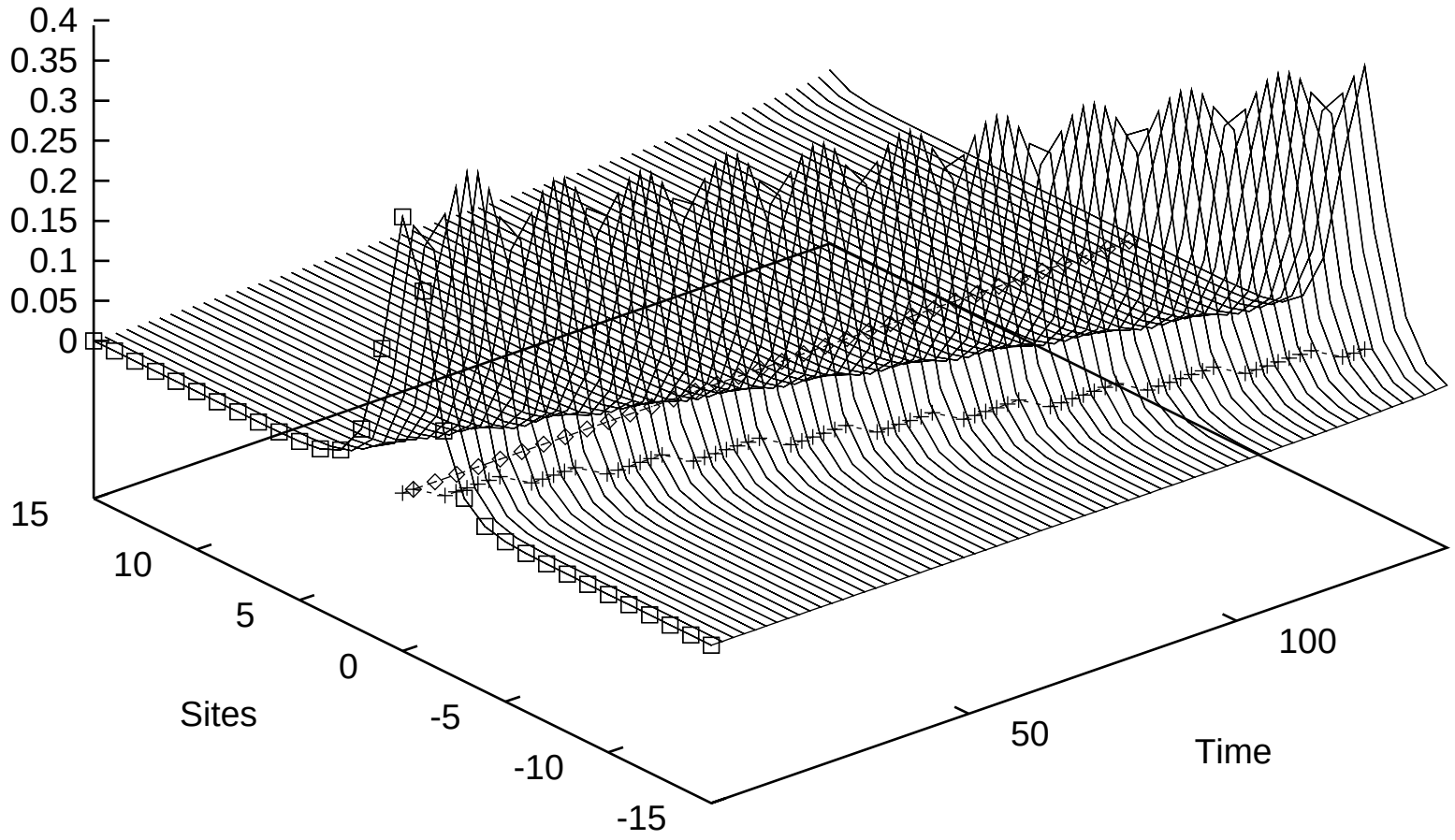
[14] J.L. Sepulchre and R.S. MacKay, preprint

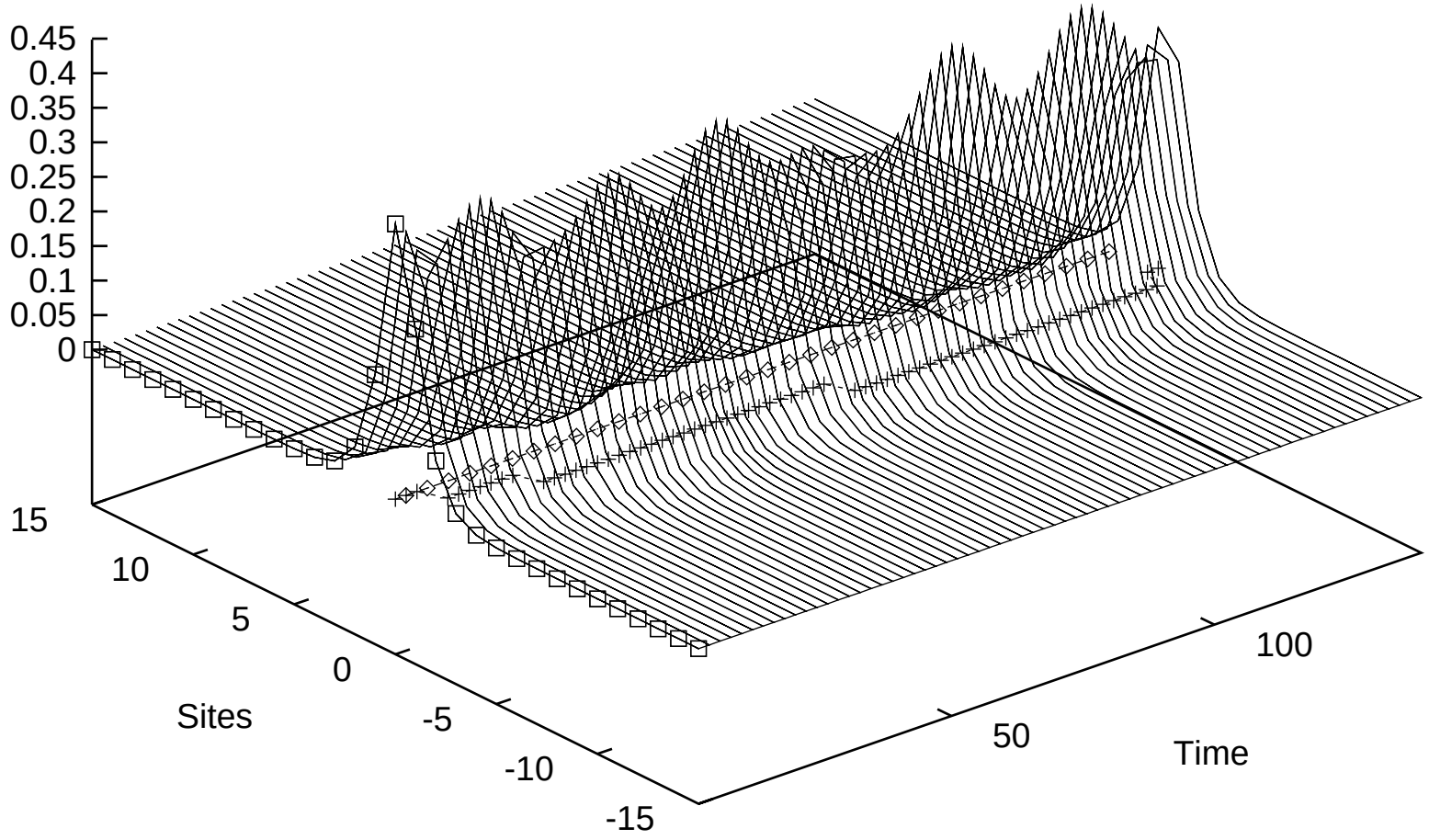
[15] Ding Chen, S. Aubry and G. Tsironis, Phys.Rev.Letts **77** (1996) 4776-4779

[16] S.Aubry and P. Quemerais, in *Singular Behavior & Nonlinear Dynamics* Ed. St. Pnevmatikos, T. Bountis & Sp. Pnevmatikos, World Scientific (1989) p.p.342-363

[17] P. Quemerais, D.K. Campbell, J.L. Raimbault and S.Aubry, Int. J. Mod. Phys. **B7**, (1993) 4289-4303

[18] L. Proville and S. Aubry, in preparation


0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
15
10
5
0
-5
-10
-15
Sites
50
100
Time


0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
15
10
5
0
-5
-10
-15
Sites
50
100
Time